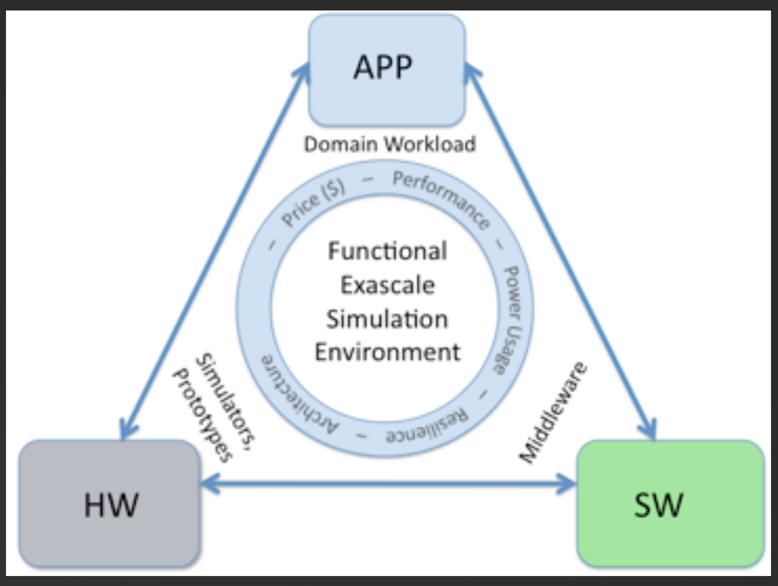
Exascale Co-design Center for Materials in Extreme Environments

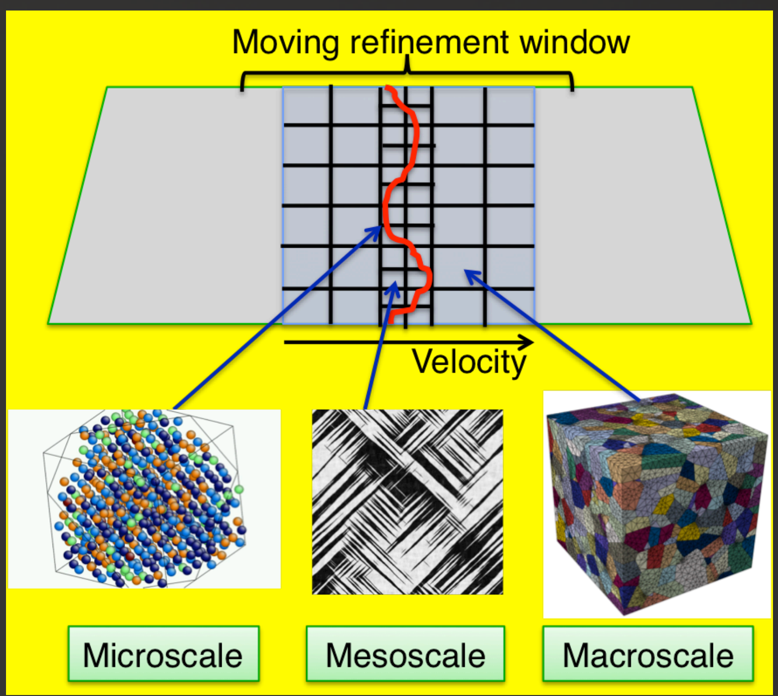
Our *goal* is to establish the interrelationships between **Application** algorithms, **Software** (programming model and middleware), and **Hardware** architectures to enable exascale-ready materials science apps in ~2020.

- In our first 18 months, we have established a set of proxy applications, and used them as a vehicle for collaboration with the DOE FastForward vendors and ASCR X-stack Computer Science research partners.
- Hackathons with AMD, IBM, Intel, and Nvidia have enabled initial assessments of emerging technologies.
- Co-design involves finding the optimal tradeoffs between algorithm, programming, and architecture choices.



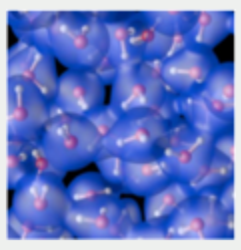
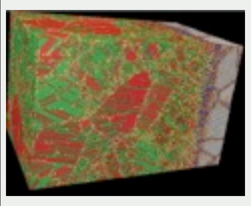
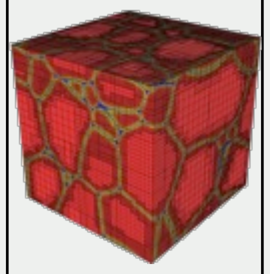
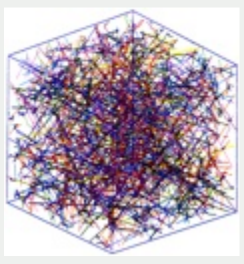
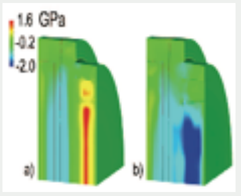
Our *strategy* is to exploit hierarchical, heterogeneous architectures to achieve more realistic large-scale simulations via an adaptive physics refinement which increases the fidelity as needed by spawning finer-scale calculations.

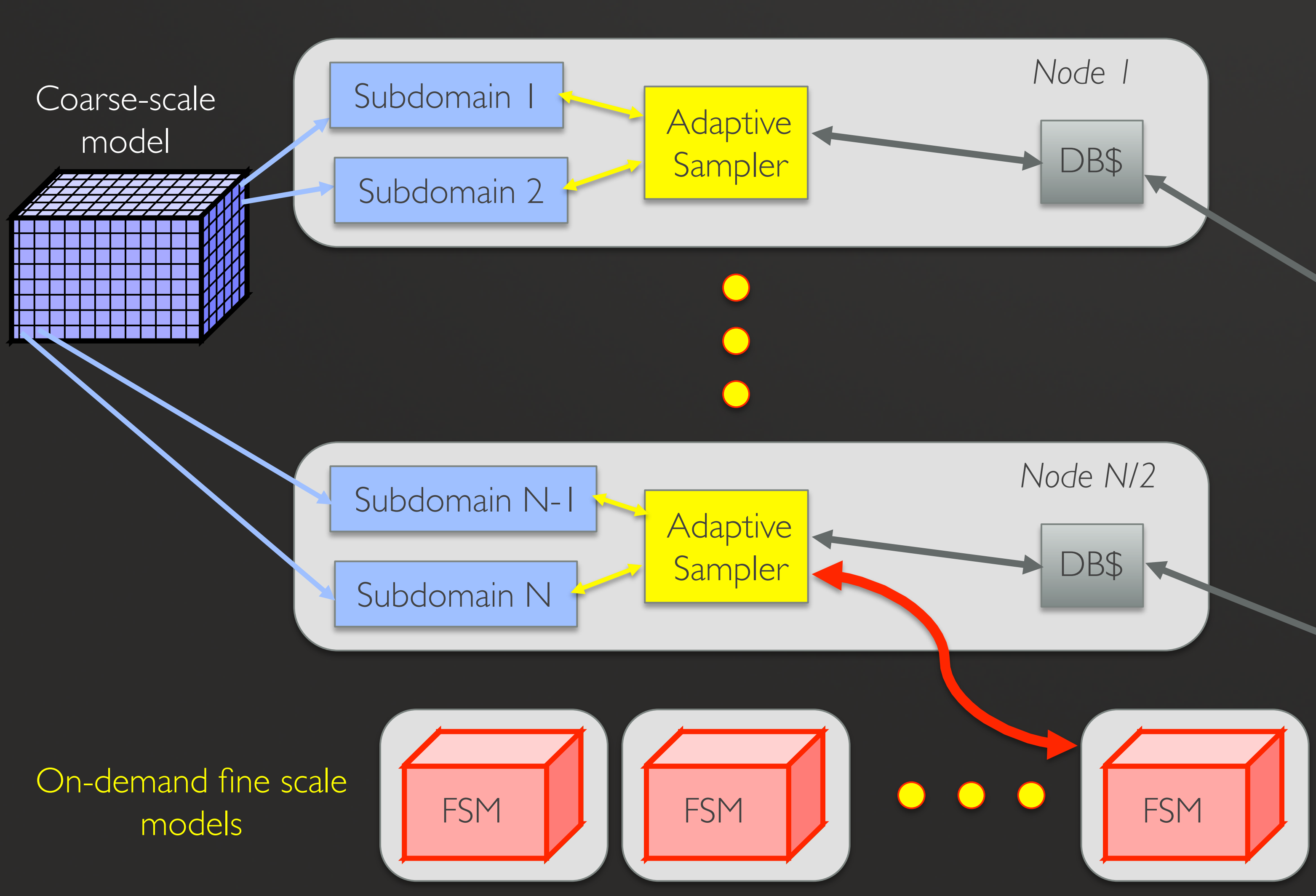
- Exascale computing will transform computational materials science by enabling the pervasive embedding of microscopic behavior into meso- and macroscale materials simulation.
- This will exploit, rather than avoid, the greatly increased levels of concurrency, heterogeneity, and flop/byte ratios on future exascale platforms.



Proxy apps representing the workflow have been an effective mechanism for:

- Exploring algorithmic choices via rapid prototyping
- Identifying language/compiler weaknesses
- Indicating bottlenecks that more complex computational workflows may have (vs. conventional benchmarks)
- Providing tractable application testbeds for new approaches to resilience, OS/runtime/execution models, power management, …
- Evaluating alternative programming models, e.g. task-based execution models & runtime systems

Ab-initio	MD	Long-time	Phase Field	Dislocation	Crystal	Continuum
Inter-atomic forces, EOS	Defects, interfaces, nucleation	Defects and defect structures	Meso-scale multi-phase evolution	Meso-scale strength	Meso-scale material response	Macro-scale material response
						
Code: Qbox/ LATTE **Motif: Particles, wavefunctions, plane wave DFT, ScaLAPACK, BLACS, and custom parallel 3D FFTs** **Prog. Model: MPI + CUDA**	**Code: SPaSM/ ddcMD/CoMD** **Motif: Particles, explicit time integration, neighbor and linked lists, dynamic load balancing, parity error recovery, and *in situ* visualization** **Prog. Model: MPI + Threads**	**Code: SEAKMC** **Motif: Particles and defects, explicit time integration, neighbor and linked lists, and *in situ* visualization** **Prog. Model: MPI + Threads**	**Code: AMPE/ CoGL** **Motif: Regular and adaptive grids, implicit time integration, real-space and spectral methods, complex order parameter** **Prog. Model: MPI**	**Code: ParaDis** **Motif: "segments" Regular mesh, implicit time integration, fast multipole method** **Prog. Model: MPI**	**Code: VP-FFT** **Motif: Regular grids, tensor arithmetic, meshless image processing, implicit time integration, 3D FFTs.** **Prog. Model: MPI + Threads**	**Code: ALE3D/ LULESH** **Motif: Regular and irregular grids, explicit and implicit time integration.** **Prog. Model: MPI + Threads**



Our scale-bridging algorithm work is improving the physics fidelity of coarse-scale models:

Bottom-up
We have developed a tractable scale-bridging proxy app (CoHMM: Co-designed Heterogeneous Multiscale Method) that represents the basic task-based modeling approach we are targeting, to begin assessment of task-based OS/runtime requirements.

Top-down
We have developed an Adaptive Sampling Proxy Application (ASPA) that represents the fine-scale query, database lookup, and kriging interpolation steps.

FUNDING AGENCY: ASCR

FUNDING ACKNOWLEDGEMENT: Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

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LA-UR-13-27513